Localization corrections and small-q phonon-mediated unconventional superconductivity in the cuprates

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(February 1, 2008)

Taking into account the first localization corrections in the electron-impurity self-energy we study the effect of non-magnetic impurities on unconventional superconductivity (SC) mediated by small-q electron-phonon scattering. We show that when van Hove singularities are close to the Fermi level making the electronic system anisotropic as in the high-T_c oxides, both the d-wave and s-wave states are sensitive to non-magnetic impurities and beyond a critical impurity concentration SC disappears in *both gap symmetry channels*. Impurity doping may induce a first order transition from d-wave to s-wave SC, but no saturation of the impuruty effect is reported due to the intrinsically anisotropic character of the localization corrections in this context.

PACS numbers: 74.25.Jb, 74.20.-z

It is now established that the pairing symmetry in the high-T_c cuprates is dominantly d-wave [1]. The most common approach associates the d-wave symmetry with a pairing mechanism involving spin fluctuations. An alternative approach has been proposed recently according to which the gap symmetry could be an energetically *marginal* parameter [2]. The basis of this last approach is the conjencture that the pairing scattering is dominated by *attractive longwavelength processes involving phonons* [2]. Small-q pairing may lead to d-wave superconductivity (SC) mediated by phonons in the cuprates, and this approach becomes particularly attractive in the light of recent experimental reports suggesting new evidence for a phonon mechanism in these compounds [3].

When forward processes dominate the pairing, there is a decorrelation tendency for SC in the various regions of the Fermi surface and gap anisotropies are driven by the anisotropies of the electronic system itself [4]. This situation has been named the *Momentum Decoupling* (MD) regime [2,4]. Depending on the details of the conventional Coulomb pseudopotential one can naturally obtain d-wave gap symmetries and it is even possible to obtain gap symmetry transitions by changing the doping or the concentration of impurities [2,5]. The presence of a significant s-wave component in the dominantly d-wave gap of YBCO is understood in the MD regime as resulting from the orthorhombic distortion of the CuO_2 planes [6] and in this context we can also fit the anisotropic pressure dependence of T_c in YBCO compounds [7]. Effectively longwavelength pairing in high-T_c compounds has been considered by many authors in different contexts eventhough in some cases it is only implicit [8]. Small-q phonon pairing has also been shown to reproduce accurately the X-shaped d-wave gap and related anomalies in $\kappa - BEDT$ organic superconductors [9].

In the MD regime, the condensation free energies of anisotropic s- and d-waves may have similar magnitude. Since non-magnetic impurities reduce more efficiently the condensation free enrgy of a d-wave gap, beyond a critical impurity density one expects that the s-wave gap may have a lower free energy and thus a d-wave to s-wave transition may be induced [5]. As a result, at sufficiently high impurity concentration, SC would be expected to be insensitive to impurities as in conventional s-wave superconductors following Anderson's theorem. However, impuirities destroy superconductivity in the cuprates and no regime of saturation of the impurity effect is observed [10]. We show here that the saturation regime is in fact never reached because in such anisotropic systems the localization corrections corresponding to the crossed impurity diagrams are *intrinsically anisotropic* and therefore Anderson's theorem do not applies.

Many studies of the effects of normal impurities in unconventional SC have been carried out especially in heavy Fermion [11] and high-T_c SC [12]. With some exceptions like in Ref. [13], the influence of realistic anisotropic bands and in particular van Hove singularities on the impurity effects has not been investigated in much detail. The first impurity self-energy diagram considered in the usual studies of SC is shown in figure 1a and the corresponding self energy is given by

$$\Sigma^{(1)}(\omega_n) = n_i V^2 \sum_{\vec{k}} \frac{1}{i\omega_n - \xi_{\vec{k}} - \Sigma(\vec{k}, \omega_n)} \qquad (1)$$

where n_i is the density of impurities and V the scattering potential. This type of self-energy diagrams cannot lead to localization and correspond to ladder diagrams in the particle-hole propagator [14]. Enhancing the concentration of impurities, the localization effects in the transport are known to occur from the series of maximally crossed diagrams [14,15] in the particle-hole propagator. In the self-energy, the localization effects manifest in the diagrams with crossed electron-impurity interaction lines. We adopt here a "perturbative" approach including only the first crossed diagram and this is what we call the first localization correction in the self-energy. We will also limit our discussion in the Born approximation. We

will focus on qualitative points that are related to the momentum dependence of these self energy corrections which are probably robust even if next order diagrams are included, because all crossed self energy diagrams are expected momentum dependent in highly anisotropic electronic systems.

The first localization correction $\Sigma^{(2)}$ that we consider here is given by (Figure 1b)

$$\Sigma^{(2)}(\vec{k},\omega_n) = n_i^2 V^4 \sum_{\vec{k}',\vec{k}''} \frac{1}{[i\omega_n - \xi_{\vec{k}'} - \Sigma(\vec{k}',\omega_n)]}$$

$$\times \frac{1}{[i\omega_n - \xi_{\vec{k}''} - \Sigma(\vec{k}'',\omega_n)]} \times$$

$$\times \frac{1}{i\omega_n - \xi_{\vec{k}'-\vec{k}''+\vec{k}} - \Sigma(\vec{k}'-\vec{k}''+\vec{k},\omega_n)} \qquad (2)$$

$\Sigma^{(2)}$ is second order in $n_i V^2$ compared to $\Sigma^{(1)}$ and our approach may be viewed as a first order expansion in $n_i V^2$ of the localization effects. The impurity scattering potential V is considered momentum independent (local) in our approach. As a result, the $\Sigma^{(1)}$ term is also momentum independent. On the other hand, $\Sigma^{(2)}$ is *momentum dependent* despite the local character of the scattering potential. Corrections of the type of $\Sigma^{(2)}$ introduce therefore an *intrinsically anisotropic* impurity scattering if the electronic system is itself anisotropic. Notice that the anisotropic character of the localization terms in anisotropic electronic systems has already been pointed out in Ref. [16]. We therefore expect a non-trivial interplay of our impurity self-energy effects with anisotropic SC that we have explored numerically.

In the superconducting state, the Dyson equation for the impurity self-energy effects reads [11]

$$\left[i\omega_n\hat{\tau}_0 - \xi_{\vec{k}}\hat{\tau}_3 - \Delta_{\vec{k}}\hat{\tau}_1 - \hat{\Sigma}(\vec{k},i\omega_n)\right]\hat{G}(\vec{k},i\omega_n) = \hat{\tau}_0 \qquad (3)$$

where $\hat{\tau}_i$ are the Pauli matrices in the usual notations. Solving the SC self-consistency problem that results from equations (1-3) is a formidable task that requires further simplifications. We adopt here a *"generalized"* Born approximation. Within this approximation we can write:

$$\tilde{\omega}_n = \omega_n + i n_i V^2 \sum_{\vec{k}'} \frac{i\omega_n}{(i\omega_n)^2 - \Delta^2_{\vec{k}'} - \xi^2_{\vec{k}'}}$$

$$+ i n_i^2 V^4 \sum_{\vec{k}',\vec{k}''} \frac{i\omega_n}{(i\omega_n)^2 - \Delta^2_{\vec{k}'} - \xi^2_{\vec{k}'}} \times$$

$$\frac{i\omega_n}{[(i\omega_n)^2 - \Delta^2_{\vec{k}''} - \xi^2_{\vec{k}''}]} \frac{i\omega_n}{[(i\omega_n)^2 - \Delta^2_{\vec{k}'-\vec{k}''+\vec{k}} - \xi^2_{\vec{k}'-\vec{k}''+\vec{k}}]} \qquad (4)$$

$$\tilde{\Delta}_{\vec{k}} = \Delta_{\vec{k}} + n_i V^2 \sum_{\vec{k}'} \frac{\Delta_{\vec{k}'}}{(i\omega_n)^2 - \Delta^2_{\vec{k}'} - \xi^2_{\vec{k}'}}$$

$$+ n_i^2 V^4 \sum_{\vec{k}',\vec{k}''} \frac{\Delta_{\vec{k}'}}{(i\omega_n)^2 - \Delta^2_{\vec{k}'} - \xi^2_{\vec{k}'}} \times$$

$$\frac{\Delta_{\vec{k}''}}{[(i\omega_n)^2 - \Delta^2_{\vec{k}''} - \xi^2_{\vec{k}''}]} \frac{\Delta_{\vec{k}'-\vec{k}''+\vec{k}}}{[(i\omega_n)^2 - \Delta^2_{\vec{k}'-\vec{k}''+\vec{k}} - \xi^2_{\vec{k}'-\vec{k}''+\vec{k}}]} \qquad (5)$$

$$\tilde{\xi}_{\vec{k}} = \xi_{\vec{k}} + n_i V^2 \sum_{\vec{k}'} \frac{\xi_{\vec{k}'}}{(i\omega_n)^2 - \Delta^2_{\vec{k}'} - \xi^2_{\vec{k}'}}$$

$$+ n_i^2 V^4 \sum_{\vec{k}',\vec{k}''} \frac{\xi_{\vec{k}'}}{(i\omega_n)^2 - \Delta^2_{\vec{k}'} - \xi^2_{\vec{k}'}} \times$$

$$\frac{\xi_{\vec{k}''}}{[(i\omega_n)^2 - \Delta^2_{\vec{k}''} - \xi^2_{\vec{k}''}]} \frac{\xi_{\vec{k}'-\vec{k}''+\vec{k}}}{[(i\omega_n)^2 - \Delta^2_{\vec{k}'-\vec{k}''+\vec{k}} - \xi^2_{\vec{k}'-\vec{k}''+\vec{k}}]} \qquad (6)$$

and the superconducting properties are obtained solving a gap equation as usually

$$\Delta_{\vec{k}} = -T \sum_{\vec{k}'} \sum_{\omega_n} \frac{\Lambda(\vec{k},\vec{k}')\tilde{\Delta}_{\vec{k}'}}{\tilde{\omega}_n^2 + \tilde{\Delta}^2_{\vec{k}'} + \tilde{\xi}^2_{\vec{k}'}} \qquad (7)$$

where $\Lambda(\vec{k},\vec{k}')$ is the pairing potential to be specified below and the fermion Matsubara frequencies are given by $\omega_n = (2n+1)\pi T$.

In the above formulation, strong-coupling effects in the pairing are neglected for the sake of keeping the calculations computationally tractable. Retardation could however interfere with the effects of disorder as discussed for isotropic cases in Ref. [17]. The electronic dispersion $\xi_{\vec{k}}$ that we consider is a tight-binding modelization of the CuO_2 planes of high-T_c cuprates that we have used previously in the study of the normal state *dc* resistivity [18]: $\xi_{\vec{k}} - E_{vH} = t_1(\cos k_x + \cos k_y) + t_2 \cos k_x \cos k_y + \frac{1}{2}t_3(\cos 2k_x + \cos 2k_y) + \frac{1}{2}t_4(\cos 2k_x \cos k_y + \cos k_x \cos 2k_y) + t_5 \cos 2k_x \cos 2k_y$ with $t_1 = -0.525$, $t_2 = 0.0337$, $t_3 = 0.0287$, $t_4 = -0.175$ and $t_5 = 0.0175$ (the lattice spacing is taken equal to one). This type of dispersion reproduces the *extended* regions of flat bands centered at the saddle points $(0, \pm\pi)$ and $(\pm\pi, 0)$ and E_{vH} is the distance in energy of the van Hove peak in the angle integrated electronic density of states from the Fermi level (when $E_{vH} = 0$ the peak in the DOS is exactly at the Fermi level [18]).

To study the effect of localization corrections in the MD regime we consider a pairing pottential similar to that in Refs. [2,4,6,7] written for small-$\mathbf{q}$ as follows

$$\Lambda(\vec{k}-\vec{p}) = -\Lambda^0 \left(1 + \frac{|\vec{k}-\vec{p}|^2}{Q_c^2}\right)^{-1} + \mu^*(\vec{q}) \qquad (8)$$

The pairing pottential is isotropic and dominated by the processes that transfer a momentum smaller than Q_c which plays the role of an effective momentum cut-off and is taken here equal to $\pi/6$ [4]. Although the pairing potential of eq. (8) is isotropic the gap obtained from equation (7) is anisotropic reflecting mainly the anisotropy of the Fermi velocity in our system [4]. The Coulomb pseudopotential μ^* is taken momentum independent and equal to $\Lambda^0/10$ so that without impurities the anisotropic d-wave solution is the one with the lowest free energy [2]. We display in Figure 2 typical d-wave and s-wave solutions that we have obtained using our kernel and our model dispersion with the extended van-Hove singularities taken exactly on the Fermi surface. In both symmetry channels the solutions are anisotropic. The largest gap values are observed in the areas around $(0, \pm\pi)$ and $(\pm\pi, 0)$ where the extended flat regions of the model dispersion are centered and the density of states is high. Density of states driven anisotropies is a key characteristic of the MD regime [2,4].

We study the evolution of the critical temperature of such states when an increasing density of impurities is introduced. We show in figure 3a a characteristic set of our results when the impurity potential is about half the bandwidth and the van Hove peak at $30meV$ below the Fermi level. One can see in figure 3a that when the concentration of impurities grows, the anisotropic s-wave state (circles) becomes rapidly more favorable than the anisotropic d-wave state (triangles). This transition has been predicted by Abrikosov [5]. Such transitions from d-wave to s-wave have also been reported as a function of the magnitude and momentum structure of the Coulomb pseudopotential using the same pairing kernel [2]. Applying a uniform magnetic field parallel to the planes (Zeeman field) may also induce gap symmetry transitions in this context [9]. This *volatility* of the gap symmetry could not be obtained in the context of a spin fluctuations pairing mechanism.

Despite the fact that at high impurity density we are in an anisotropic s-wave state the critical temperature is continuously reduced when we further enhance the concentration of impurities. No saturation regime is reached in qualitative agreement with the experiments on high-$T-c$ cuprates. Like the d-wave state, the s-wave state *collapses* beyond a critical concentration of impurities. This unexpected behavior is due to the proximity of the van Hove singularity to the Fermi level as can be clearly seen in Fig. 3b where we report results in the s-wave channel as a function of the distance of the van Hove peak from the Fermi level.

The momentum dependence of the crossed diagram corrections as well as the density of states driven anisotropic SC induced by the singular at small-q kernel we are using [4] play a crucial role in eliminating the saturation of the impurity effect. In fact, we have performed calculations in which the terms related to $\Sigma^{(2)}$ were set equal to zero and the resulting behavior is qualitatively similar to that obtained including $\Sigma^{(2)}$ but with the van-Hove singularities far from the Fermi level. Moreover, the impurity effects in the s-wave channel depend on the magnitude of Q_c, being more drastic when Q_c is reduced illustrating the importance of density of states driven anisotropies in the MD regime [4,2].

A quantitative comparison of our calculations with the experiments at that level of approximation is out of question and the quantitative dependence of our results on the various parameters will be explored elsewhere. The present results clearly demonstrate that in anisotropic systems, the interplay of large concentrations of normal impurities and unconventional superconductivty may be highly non trivial and extrapolation of ideas based on Anderson's theorem should be made cautiously. When van-Hove singularities and density of states driven anisotropies are in game as in the MD regime, a saturation regime of the impurity effects on SC is never reached. As the density of impurities grows the inclusion of localization corrections is unavoidable and these last corrections are intrinsically anisotropic in this regime preventing the aplicability of Anderson's theorem.

I acknowledge enlightening comments by Boris Altshuler on the aplicability of Anderson's theorem in the presence of effectively momentum dependent scattering.

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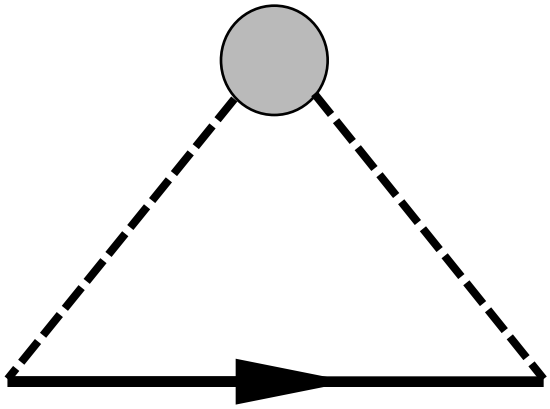
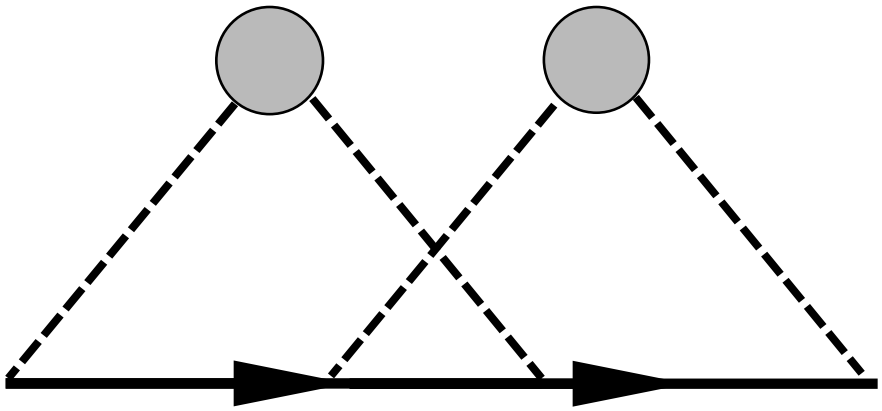
Figure Captions

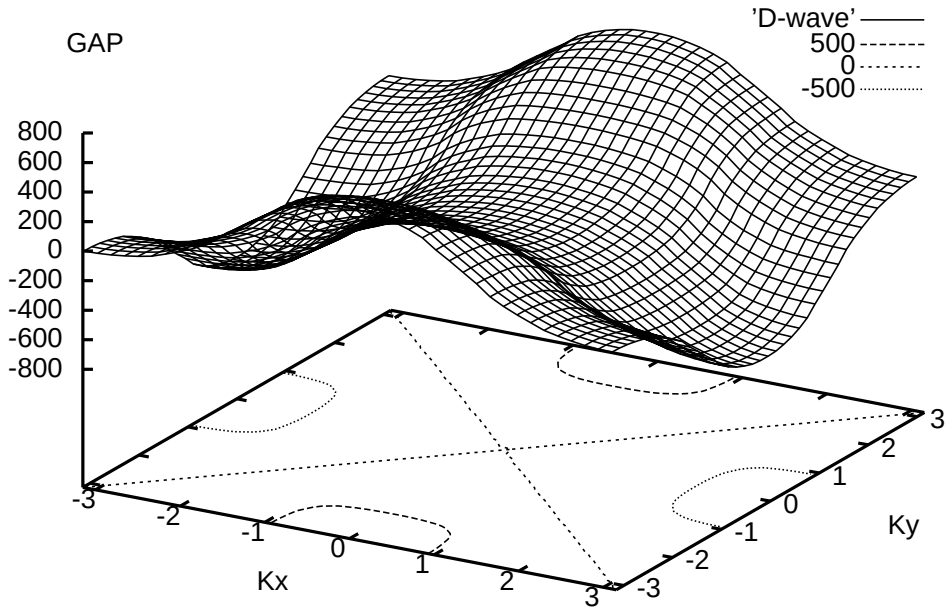
Figure 1: Electron impurity self-energy diagrams. In (a) the self-energy effects considered in the usual Born approximation and in (b) the first localization corrections.

Figure 2: Typical d-wave (a) and s-wave (b) gap solutions over the first Brillouin zone of our model dispersion obtained using a pairing potential having the form of Eq. (8) as described in the texte.

Figure 3: (a) The ratio T_c/T_c^d as a function of the density of impurities (T_c^d is the critical temperature of the d-wave gap without impurities). The d-wave solution dominates without impurities. As the density of impurities grows, the T_c of the s-wave (circles) becomes higher than that of the d-wave (triangles) and s-wave becomes the physical state of the system. In both symmetries T_c is reduced continuously with impurity doping towards zero. (b) Evolution of T_c in the s-wave channel for three characteristic cases of distance of the van-Hove peak to the Fermi level: $E_{vH} = 30meV$ (circles), $60meV$ (squares) and $90meV$ (triangles).



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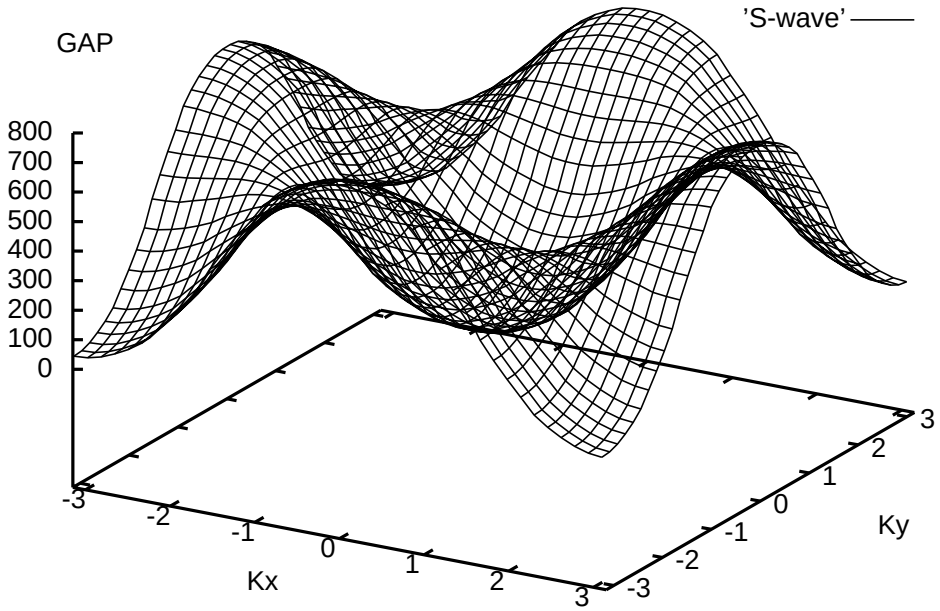
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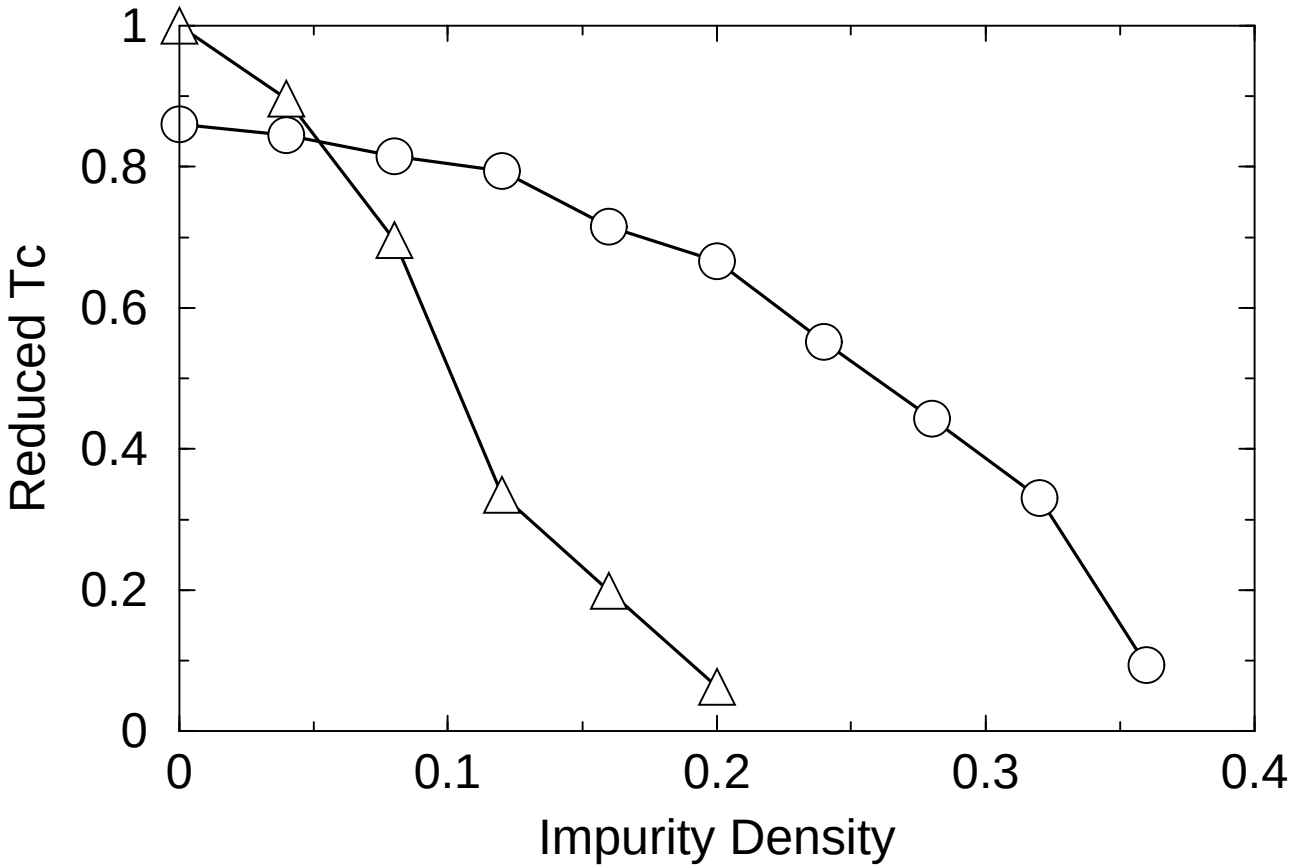
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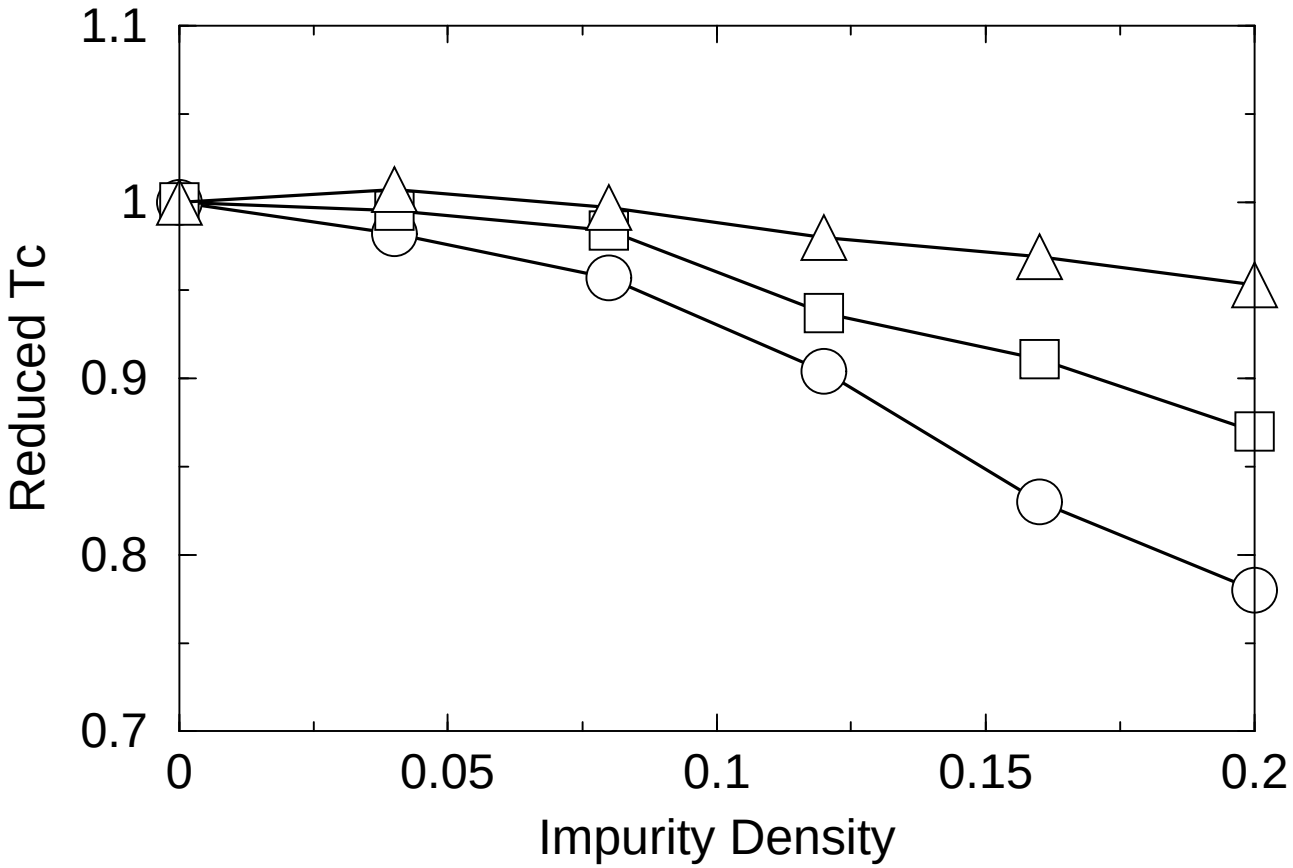
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